STRUCTURAL CHEMISTRY

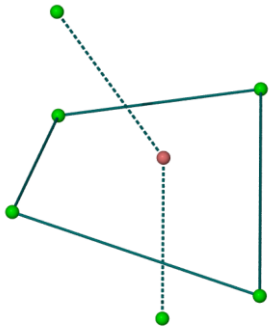
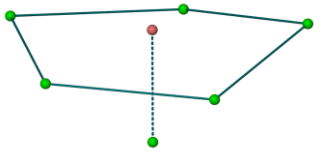
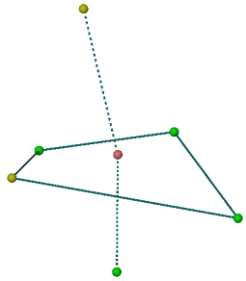
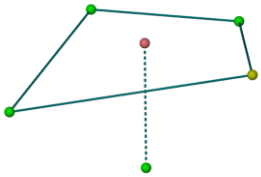
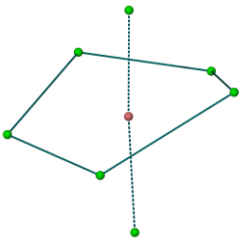
Volume 77 (2021)

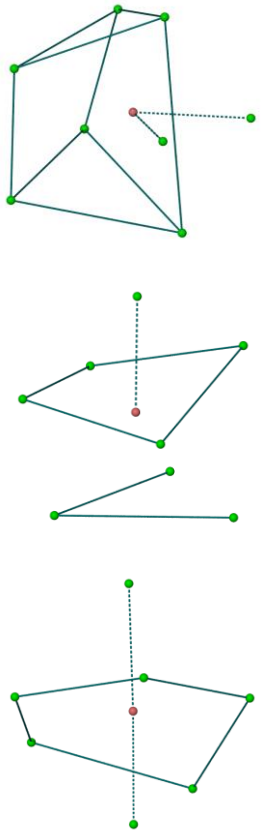
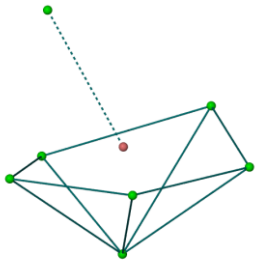
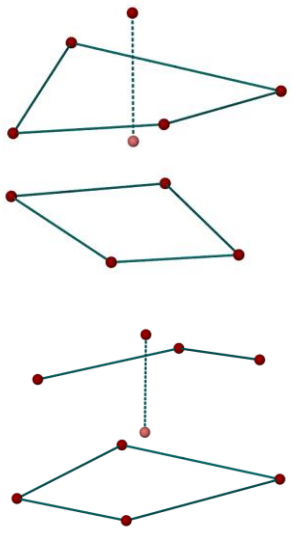
Supporting information for article:

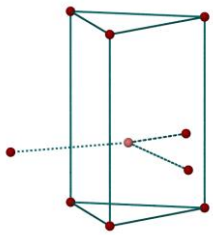
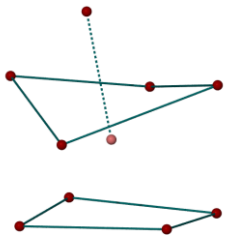
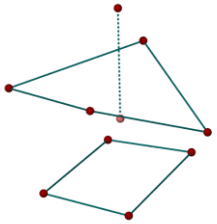
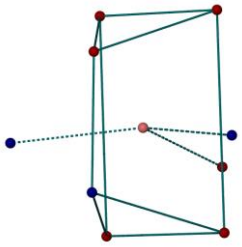
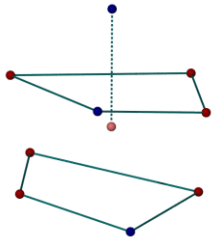
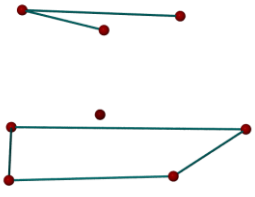
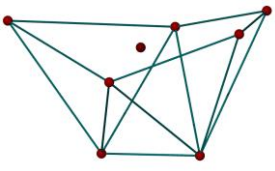
Resolvable polymorphism in an intergrowth of two modifications of tris(diethyldithiocarbamato)antimony

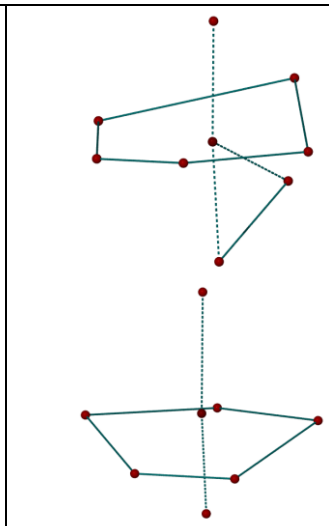
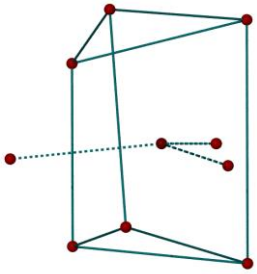
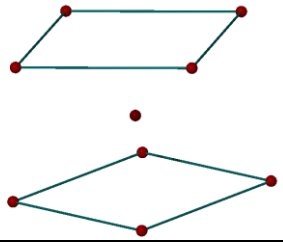
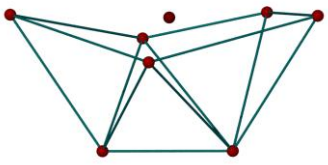
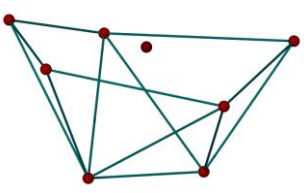
Seik Weng Ng

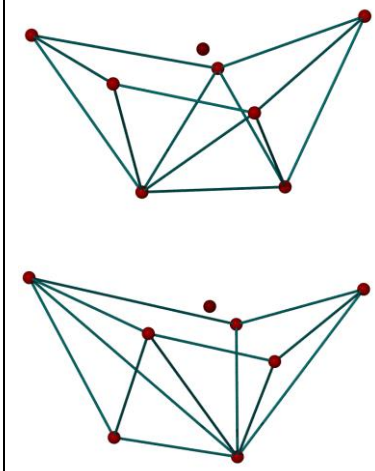
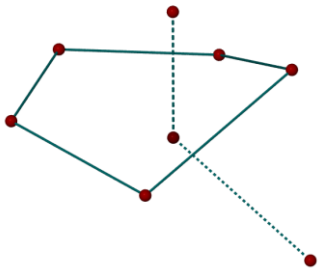
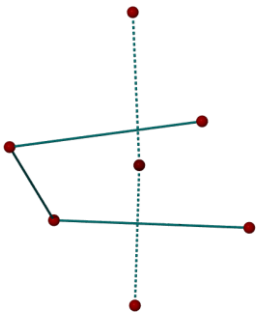
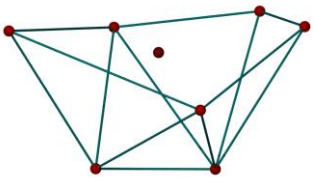
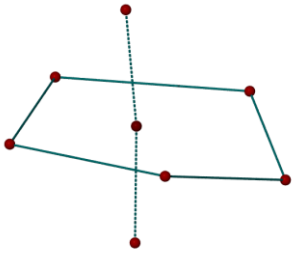
Table S1. Polyhedral symbols for coordination geometries for pairs of Sb(III), Bi(III) and Pb(II) polymorphs

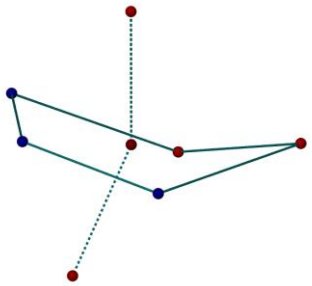
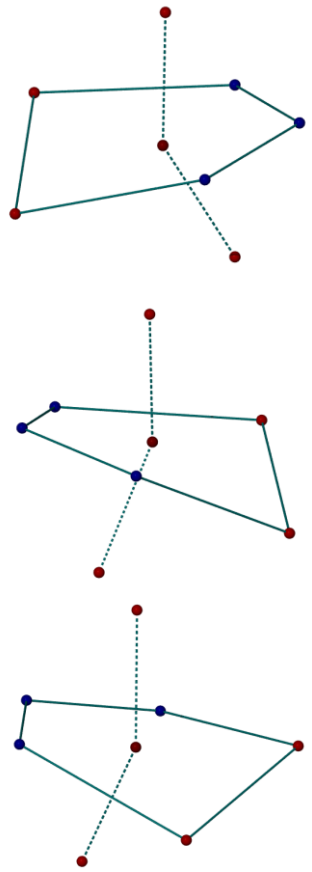
Formula	**Space group**	**Polyhedron**	**Polyhedral symbol**	**Reference**
$Sb(S_2CNMe_2)_3$	*P*-1		ψ-OFC-7	This work
$Sb(S_2CNMe_2)_3$	$P2_1/c$		ψ-PBPY-7	This work; Que *et al.*, 2009; Raston & White, 1976
$SbCl(S_2CNMe_2)_2$	$P2_1/c$		ψ-OFC-7	Ozturk *et al.*, 2014
$SbCl(S_2CNMe_2)_2$	$P2_1/c$		ψ-OC-6	Ozturk *et al.*, 2014
$Bi(S_2CN^nBu_2)_3$ Bi at (0.3910, 0.836, 0.8604) Bi at (0.6600, 0.7342, 0.8780)	*P*-1		PBPY-7 ψ-TPRS-9	Gowda *et al.*, 2017

Bi at (0.3526, 0.3164, 0.6268) Bi at (0.6168, 0.2164, 0.6466)			ψ-SAPRS-9 PBPY-7	
$Bi(S_2CN^nBu_2)_3$	$P2_1/n$, $P2_1/c$		ψ-DD-8	Gowda *et al.*, 2017; Sun *et al.*, 2012
$Bi(O_2CPh)_3$ Bi at (0.1629, 0.3068, 0.7174) Bi at (0.6650, 0.2569, 0.7979)	$P2_1/m$		 SAPRS-9 ψ-SAPRS-9	Rae *et al.*, 1998

$Bi(O_2CPh)_3$	*R*3		TPRS-9	Tumanov *et al.*, 2010
$Bi(C_{10}H_3O_8)$	*P*-1		SAPRS-9	Feyand *et al.*, 2013
$Bi(C_{10}H_3O_8)$	$P2_1/a$		SAPRS-9	Feyand *et al.*, 2013
$Bi(C_6H_4NO_2)_3$	$P2_1$		TPRS-9	Anjaneyulu & Swamy, 2011 Callens *et al.*, 2008
$Bi(C_6H_4NO_2)_3$	$P2_1/n$		SAPRS-9	Anjaneyulu *et al.*, 2010
$Pb(C_2H_3O_2)_2$	$P2_1$		ψ-SAPR-8	Martínez-Casado *et al.*, 2016
$Pb(C_2H_3O_2)_2$	$P2_1/m$		ψ-DD-8	Martínez-Casado *et al.*, 2016

$Pb(C_4H_4O_4)$ Pb at (0.0143, 0.1882, 0.3053) Pb at (0.5027, 0.0629, 0.2691)	*P*2$_1$/*c*		DD-8 PBPY-7	Foremann *et al.*, 2001
$Pb(C_4H_4O_4)$	*P*2$_1$/*c*		TPRS-9	Dhanya *et al.*, 2011; Jiao *et al.*, 2009
$Pb(C_4O_4)$	*Cmma*	No coordinates		Bataille *et al.*, 2011
$Pb(C_4O_4)$	*I*4/*mcm*		SAPR-8	Bataille *et al.*, 2011
$Pb_2(H_2O)(C_{10}H_{10}O_5)$ Pb at (0.3773, 0.3572, 0.8661) Pb at (0.6352, 0.1153, 0.6348)	*P*-1	 	Ψ-DD-8 Ψ-DD-8	Yang *et al.*, 2011

$Pb_2(H_2O)(C_{10}H_{10}O_5)$ Pb at (0.4549, 0.0386, 0.8012) Pb at (-0.0002, 0.0821, 1.0736)	$P2_1$		Ψ-DD-8 Ψ-DD-8	Yang *et al.*, 2011
$Pb(C_9H_{17}O_2)_2$	*P*-1		Ψ-DD-8	Martínez-Casado *et al.*, 2017
$Pb(C_9H_{17}O_2)_2$			Ψ-PBPY-7	Martínez-Casado *et al.*, 2017
$Pb(C_{10}H_{19}O_2)_2$	*P*-1		Ψ-DD-8	Martínez-Casado *et al.*, 2017
$Pb(C_{10}H_{19}O_2)_2$	$P2_1/c$		Ψ-PBPY-7	Martínez-Casado *et al.*, 2017

$Pb(ClO_4)_2(C_{15}H_{11}N_3)$	*C*2/*c*		Ψ-DD-8	Engelhardt *et al.*, 1996
$Pb(ClO_4)_2(C_{15}H_{11}N_3)$ Pb at (0.2958, 0.5810, 0.1432) Pb at (0.1058, 0.4175, 0.0599) Pb at (0.5000, 0.4166, 0.2500)	*C*2/*c*		Ψ-DD-8 Ψ-DD-8 Ψ-DD-8	Blake *et al.*, 2009

Current cell
10.0838(8) 14.4060(11) 17.3284(13) 89.988(6) 80.409(6) 75.158(7) 2396.9(3)
Lattice reduction
selected cell
10.0838 14.4060 17.3283 89.9877 80.4084 75.1581 aP 31
reduced cell
10.0838 14.4060 17.3283 89.9877 80.4084 75.1581 2396.9
Twin information
1: 10.0843 14.4065 17.3285 89.989 80.409 75.158 2397.1
2: 12.4491 13.5099 14.6928 90.065 99.907 89.996 2434.3
1: Total: 3866(57.3%) Separate: 3789(56.2%) Overlapped: 77(1.1%)
2: Total: 2083(30.9%) Separate: 2006(29.7%) Overlapped: 77(1.1%)
Unindexed: 871 (12.9%)

PEAK TABLE
Peak hunting table
UB fit with 3866 obs out of 6743 (total:6743,skipped:0) (57.33%)

INSTRUMENT MODEL
Goniometer
beam: 0.05620 alpha: 50.10981 beta: -0.01496
om zero: 0.30814 th zero: 0.11714 ka zero: 0.32714
Detector
x-rot: 0.24574 y-rot: -0.28630
x-cen: 1022.21618 y-cen: 1035.78307 distance: 75.03628
Wavelength Mo (Ang): A1 0.70930 A2 0.71359 B1 0.63229

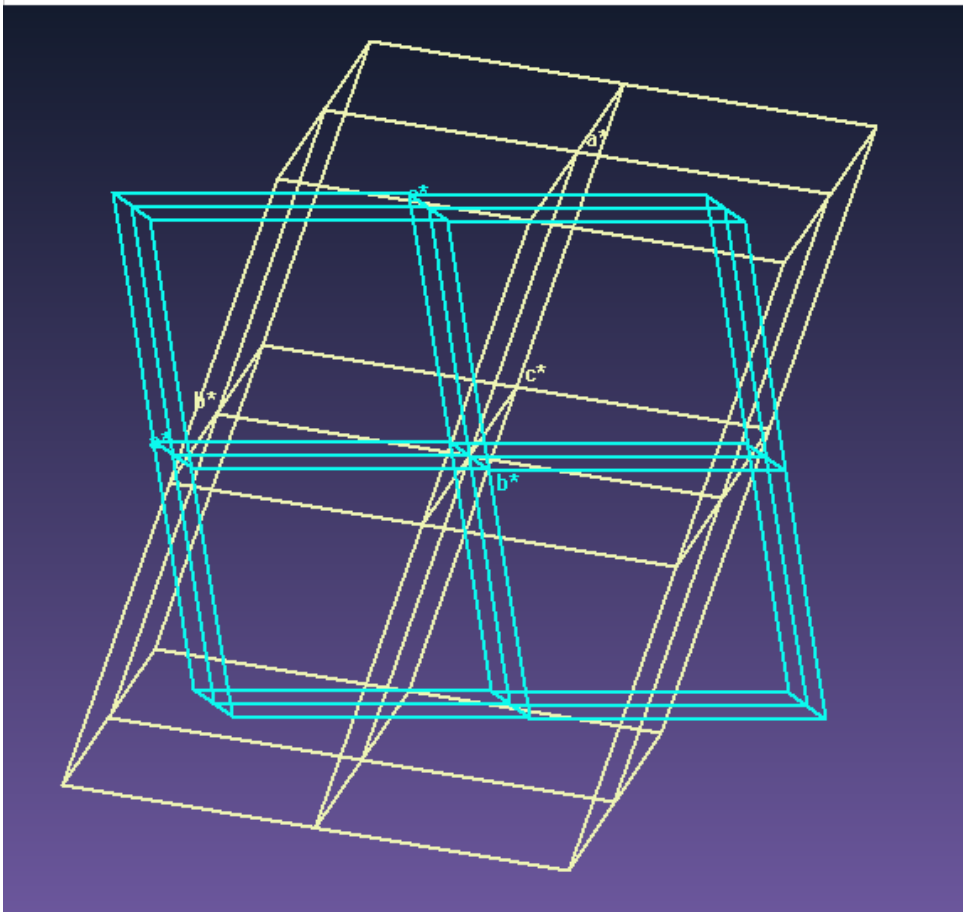


Fig. S1